Newton's Method I

Roots and Stationary Points of Univariate Scalar Functions

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Informatik 12:
Software and Tools for Computational Engineering

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Outline

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Objective and Learning Outcomes

Objective

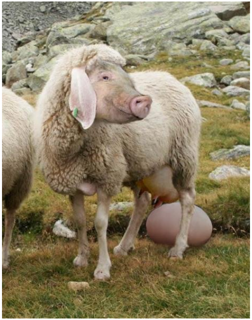
- Introduction to Newton's method for scalar functions.

Learning Outcomes

- You will understand
  - roots of nonlinear functions
  - linearization
  - convergence
  - stationary points and local optima
- You will be able to
  - implement Newton's method
  - investigate convergence of Newton's method.

Outline

The solution of linear equations amounts to simple scalar division. The solution of nonlinear equations can be challenging.



"Egg-Laying, Wool-Bearing, Milk-Giving Sow"
©Georg Mittenecker @ Wikipedia

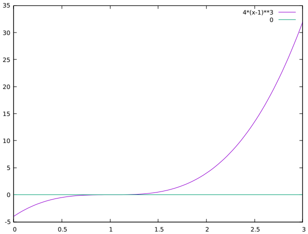
Many numerical methods for nonlinear problems are built on local (at $\tilde{x}$) replacement of the target function with a linear (affine; in Δx) approximation derived from the truncated Taylor series expansion and "hoping" that

$$f(\tilde{x} + \Delta x) \approx f(\tilde{x}) + f'(\tilde{x}) \cdot \Delta x \ ,$$

i.e, hoping for a reasonably small remainder.

The solution of a sequence of linear problems is then expected to yield an iterative approximation of the solution to the nonlinear problem. Newton's method is THE example.

Let $y = f(x)$ be continuous within a neighborhood $x + \Delta x$ of x taking values $f(x)$ and $f(x + \Delta x)$ at the endpoints of the interval. Then f takes all values between $f(x)$ and $f(x + \Delta x)$ over the same interval.



If $f(x)$ and $f(x + \Delta x)$ have different signs, then f has a root within the interval bounded by x and $x + \Delta x$, i.e, $\exists \tilde{x} : f(\tilde{x}) = 0$.

The simplest possible root finding algorithm follows from iterative / recursive bisection of the the interval $[x, x + \Delta x]$.

Unfortunately, the bisection algorithm converges slowly and does not generalize to higher dimensions. Hence, we are going to investigate superior alternatives.

Note: $\tilde{x}$ not necessarily unique; f can take values outside of $[f(x), f(x + \Delta x)]$

Outline

Consider a nonlinear equation $y = f(x) = 0$ at some (starting) point x.

Building on the assumption that $f(x + \Delta x) \approx f(x) + f'(x) \cdot \Delta x$ the root finding problem for f can be replaced locally by the root finding problem for the linearization

$$\bar{f}(\Delta x) = f(x) + f'(x) \cdot \Delta x \ .$$

The right-hand side is a straight line intersecting the y-axis in $(\Delta x = 0, \bar{f}(\Delta x) = f(x))$.

Solution of

$$\bar{f}(\Delta x) = f(x) + f'(x) \cdot \Delta x = 0$$

for Δx yields

$$\Delta x = -\frac{f(x)}{f'(x)}$$

implying $f(x + \Delta x) \approx 0$.

If the new iterate is not close enough to the root of the nonlinear function, i.e, $|f(x+\Delta x)| > \epsilon$ for some measure of accuracy of the numerical approximation $\epsilon > 0$, then it becomes the starting point for the next iteration yielding the recurrence

$$x = x - \frac{f(x)}{f'(x)}$$

Convergence of this Newton[-Raphson] method is not guaranteed in general. Damping of the magnitude of the next step may help.

$$x = x - \alpha \cdot \frac{f(x)}{f'(x)} \quad \text{for } 0 < \alpha \leq 1 \, .$$

The damping parameter α is often determined by line search (e.g, recursive bisection yielding $\alpha = 1, \; 0.5, \; 0.25, \; \ldots$) such that decrease in absolute function value is ensured.

Newton's Method

Implementation

```
template<typename T> T f(const T &x);
template<typename T> T dfdx(const T &x);

template<typename T>
void solve(T& x, const T& eps) {
  while (fabs(f(x))>eps) x-=f(x)/dfdx(x);
}

int main(int, char *v[]) {
  double x=std::stof(v[1]);
  solve(x,1e-12);
  std::cout << "x=" << x << std::endl
            << "f(x)=" << f(x) << std::endl
            << "dfdx(x)=" << dfdx(x) << std::endl
  return 0;
}
```

Newton's method can be regarded as a fixed point iteration

$$x = g(x) = x - \frac{f(x)}{f'(x)} \ .$$

If at the solution

$$|g'(x)| < 1 \ ,$$

then there exists a neighborhood containing values of x for which the fixed-point iteration converges to this solution.

The convergence rate of a fixed-point iteration grows linearly with decreasing values of $|g'(x)|$.

For $|g'(x)| = 0$ we get at least quadratic convergence; cubic for $|g'(x)| = |g''(x)| = 0$ and so forth.

Newton's method becomes

$$x = g(x) = x - \frac{f(x)}{f'(x)}$$

yielding

$$g'(x) = f(x) \cdot \frac{f''(x)}{(f'(x))^2} \; .$$

At the solution $f(x) = 0$ implies $g'(x) = 0$. Assuming a simple root ($f(x) = 0$, $f'(x) \neq 0$) the second derivative of g becomes equal to

$$g''(x) = f'(x) \cdot \frac{f''(x)}{(f'(x))^2} + \underbrace{f(x)}_{=0} \cdot (\ldots)$$

implying quadratic convergence within the corresponding neighborhood of the solution if $f''(x) \neq 0$ as well as convergence after a single iteration for linear f.

Let $f(x) = \cos(x)$. from

$$x = g(x) = x - \frac{f(x)}{f'(x)} = x - \frac{\cos(x)}{-\sin(x)}$$

follows

$$g'(x) = f(x) \cdot \frac{f''(x)}{(f'(x))^2} g'(x) = \cos(x) \cdot \frac{-\sin(x)}{(\cos(x))^2} \; .$$

At $\tilde{x} = 1$ we get $|g'(x)| \approx 0.41$ and hence convergence to the nearest root at $\frac{\pi}{2} \approx 1.57$.

At $\tilde{x} = 3$ we get $|g'(x)| \approx 49.21$ suggesting divergence. However, the second iterate $\tilde{x} \approx -4.02$ yields $|g'(x)| \approx 0.69$ resulting in convergence to the root closest to -4.02, that is, $-\frac{3 \cdot \pi}{2} \approx -4.71$.

Let $y = f(x)$ be twice continuously differentiable over the domain of interest.

- $\tilde{x}$ is a stationary point (necessary condition for local optimality) of f if

$$f'(\tilde{x}) \equiv \frac{df}{dx}(\tilde{x}) = 0$$

- $\tilde{x}$ is a local minimum (sufficient condition for local optimality) of f if

$$f''(\tilde{x}) \equiv \frac{d^2 f}{dx^2}(\tilde{x}) > 0 \quad \text{(strict convexity)}$$

- $\tilde{x}$ is a local maximum (sufficient condition for local optimality) of f if

$$f''(\tilde{x}) \equiv \frac{d^2 f}{dx^2}(\tilde{x}) < 0 \quad \text{(strict concavity)}$$

$f'' = 0$ indicates a non-simple stationary point.

Consider the nonlinear optimization problem

$$\min_{x \in R} f(x)$$

for $f : R \rightarrow R$.

Starting from some initial estimate for the stationary point $\tilde{x}$ the steepest descent method iteratively takes steps into descent directions. In the scalar case the choice is between stepping toward $-\infty$ or ∞.

The first derivative $f'(x)$ indicates local increase $(f'(\tilde{x}) > 0)$ or decrease $(f'(\tilde{x}) < 0)$ of the the function value.

Aiming for decrease the next step should be toward $-\infty$ if $f' > 0$ or toward ∞ if $f' < 0$. No further local decrease in the function value can be achieved for $f' = 0$ (necessary optimality condition).

The step size is typically damped in order to ensure continued progress toward $\min_{x \in R} f(x)$ yielding the recurrence

$$x := x - \alpha \cdot f'(x) \quad \text{while } |f'(x)| > \epsilon$$

Comments on line search apply as above.

Validation of a local minimum at $\tilde{x}$ requires $f''(\tilde{x}) > 0$. Similarly, a local maximum is found if $f''(\tilde{x}) < 0$.

Steepest Descent

Implementation

```
template<typename T> T f(const T &x);
template<typename T> T dfdx(const T &x);
template<typename T> T ddfdxx(const T &x);

template<typename T>
void solve(T& x, const T& eps) {
  T g=dfdx(x), y=f(x), y_prev;
  while (fabs(g)>eps) {
    y_prev=y;
    double alpha=2.;
    while (y_prev<=y&&alpha>eps) {
      T x_trial=x; alpha/=2;
      x_trial-=alpha*g; y=f(x_trial);
    }
    x-=alpha*g; g=dfdx(x);
  }
}
```

Consider the nonlinear optimization problem

$$\min_{x \in R} f(x)$$

for $f : \mathbf{R} \to \mathbf{R}$.

Application of Newton's method to

$$f'(x) = 0$$

yields

$$x = x - \frac{f'(x)}{f''(x)} \; .$$

Comments on convergence and line search apply as above.

Validation of a local minimum at $\tilde{x}$ requires $f''(\tilde{x}) > 0$. Similarly, a local maximum is found if $f''(\tilde{x}) < 0$.

Local Optima: Implementation

```
template<typename T> T f(const T &x);
template<typename T> T dfdx(const T &x);
template<typename T> T ddfdxx(const T &x);

template<typename T>
void solve(T& x, const T& eps) {
  while (fabs(dfdx(x))>eps)
    x-=dfdx(x)/ddfdxx(x);
}
```

Outline

Objective and Learning Outcomes

Recall
- Linearization
- Intermediate Value Theorem

Newton's Method
- Roots of Nonlinear Equations
- Stationary Points and Local Optima

Summary and Next Steps

Summary

- Newton's method for scalar functions
- roots of nonlinear equations
- stationary points and local optima

Next Steps

- Inspect sample code.
- Run further experiments.
- Continue the course to find out more ...